

Materials Model Development

ASC Review

LA-UR-03-2016



Los Alamos

ASC Materials & Physics Program

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Program Manager

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Project Leader



Program Guidance

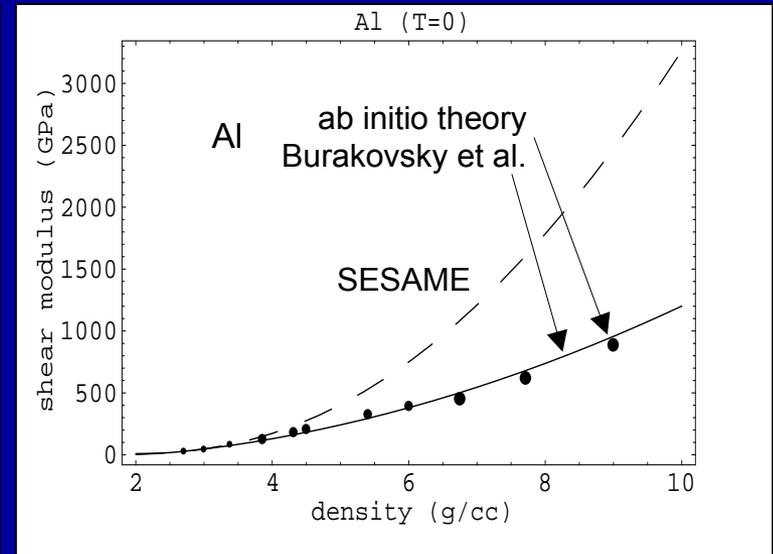
- Atomistic Modeling (Kober, Kress)
- Meso-scale Modeling (Albers, Preston)
- Macro-scale Modeling (Maudlin)
- Code Implementation (Maudlin)

Program Objectives

- Develop Materials Models
 - Physically-Based
 - Predictive
 - Numerically Robust
 - Computationally Efficient
 - Validated Models
 - ASC Code Compatible
 - Code Implementation
 - Incremental Improvements

Incremental Improvements in Materials Modeling

- Improve Existing Standard of Materials Models / Implement Models as Become Available (e.g.):
 - Materials Moduli
 - Rate-Dependent Plasticity
 - Failure
 - Steinberg-Guinan - MTS, PTW
 - Isotropic - Anisotropic
- Failure
 - P_{\min} - Ductile / Brittle Failure



Model Development

Develop Models that Capture the Physical Aspects for Materials and Regimes of Interest

- Phenomena

- High-rate plasticity
- Anisotropy
- Failure (ductile/brittle)
- Phase Transformations
- Crystal Reorientation
- Friction

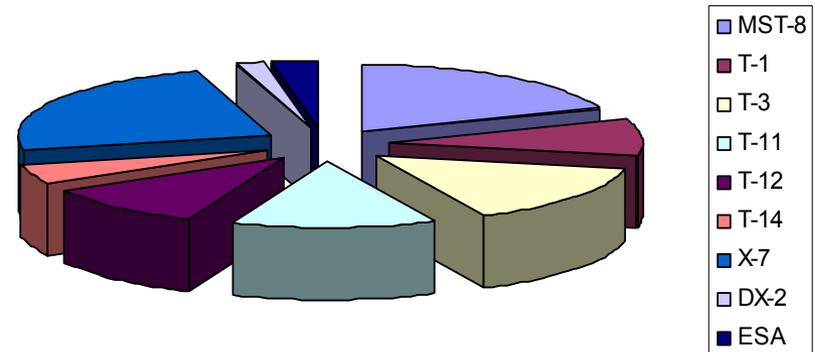
- Materials

- Metals (Pu, U, Be, ...)
- Polymers (estane,...)
- Composites
- High-Explosives
- Foams
- Surrogate Mat'ls

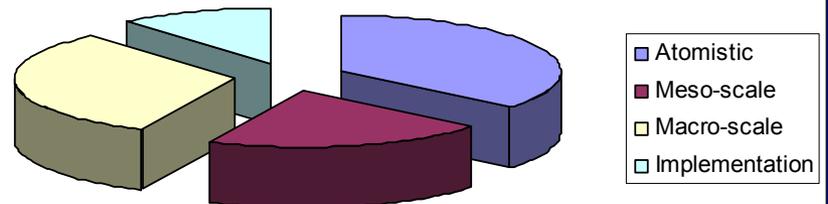
Funding Profile

- Multi-Division Effort
- Approximately 30 TSM's
- Approximately 20 FTE's
- Leveraged Program

Group Funding



Effort Funding



Coordinated Program

- Leveraged
 - DOE/DoD MOU
 - LDRD
 - BES
- Modeling Collaborations
 - ASC EOS Program
 - ASC HE Program
 - DOE / DoD MOU
- Experimental Collaborations
 - Hydro-Phase Program
 - DOE / DoD MOU

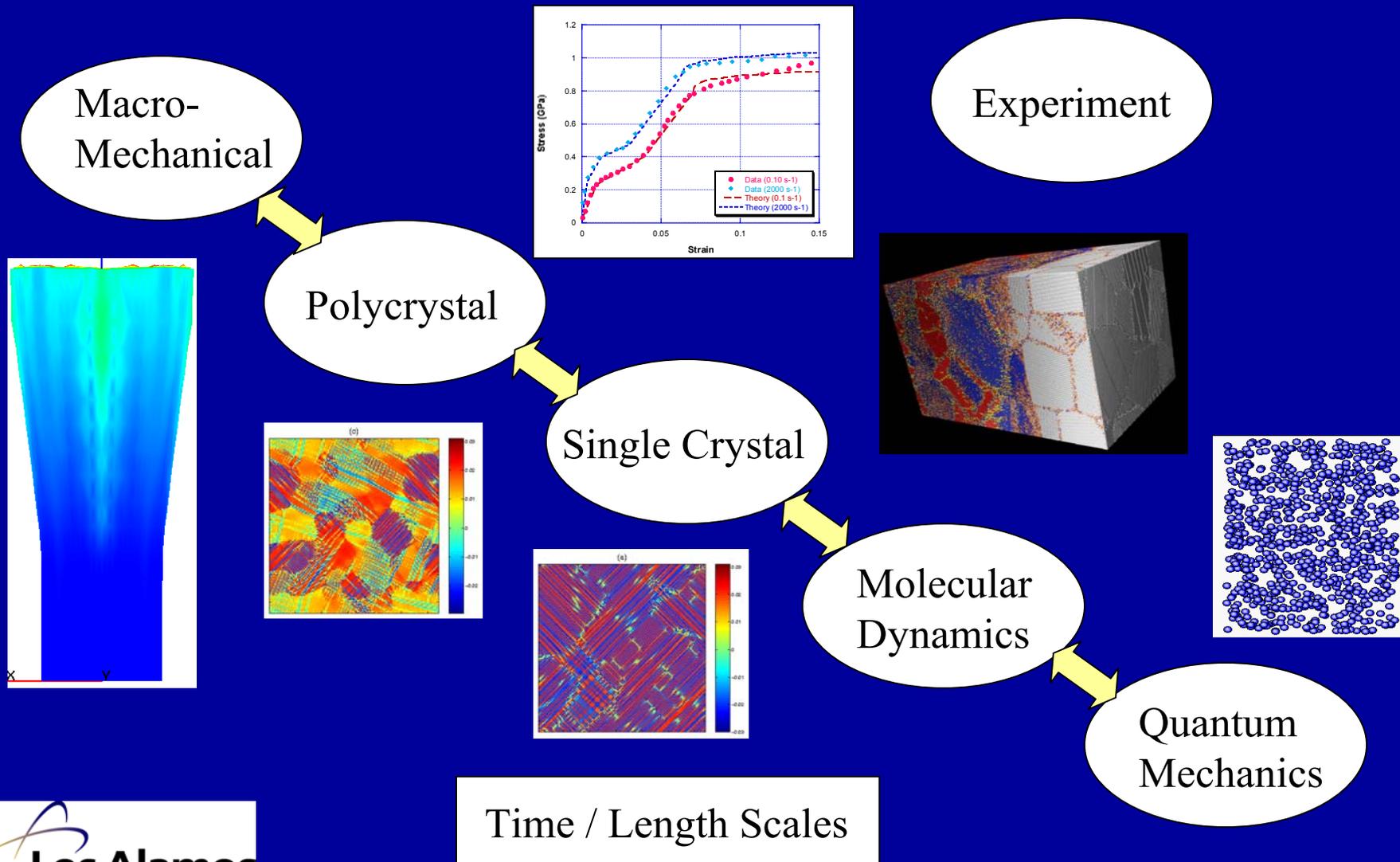
Program Customers

- Weapons Design & Applications
- ASC Code Development Programs
- Case Dynamics Program
- Experimental Design & Analysis
- Weapons Safety & STS (General Models)
- Enhanced Surveillance

Program Outline

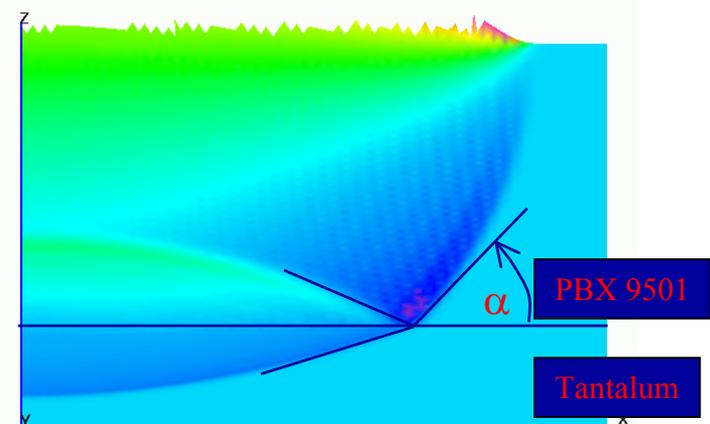
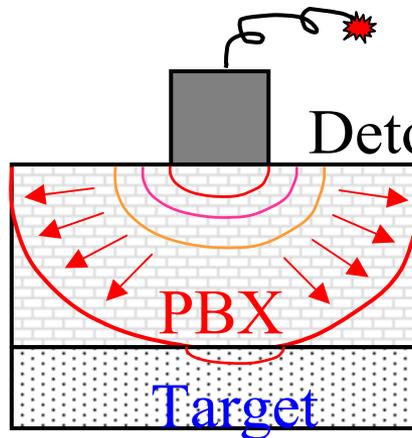
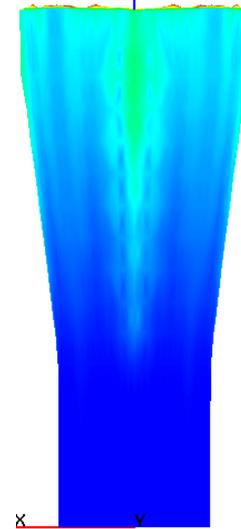
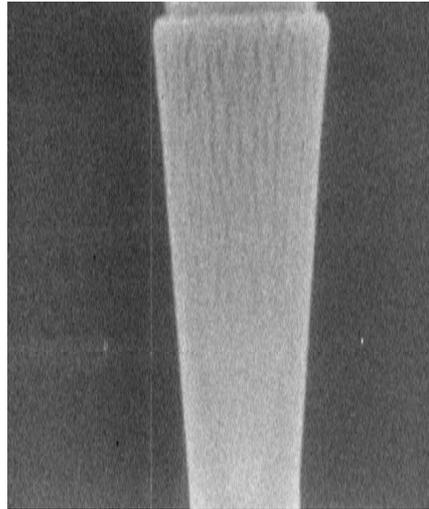
- Engineering Code Implementation
- Macro-Mechanical Model Development
- Meso-Scale Model Development
- Single / Poly-Crystal Models
- Molecular Dynamics
- Quantum Simulations
- Atomistic Potentials

Multi-Length Scale Approach



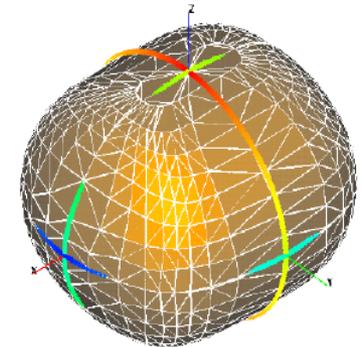
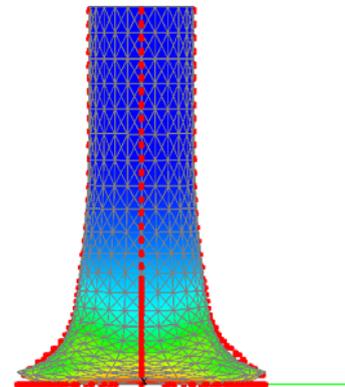
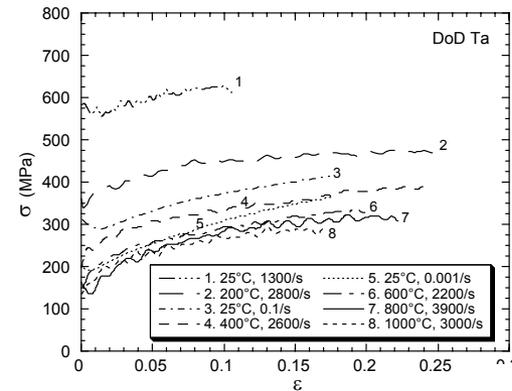
Code Implementation

- Shavano Project
- Blanca Project
- Antero Project
- Dyna
- Abaqus
- EPIC
 - Development



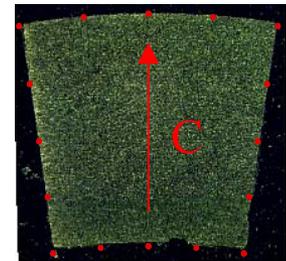
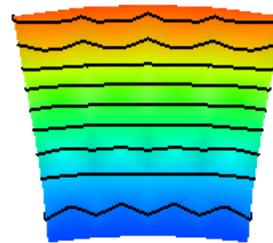
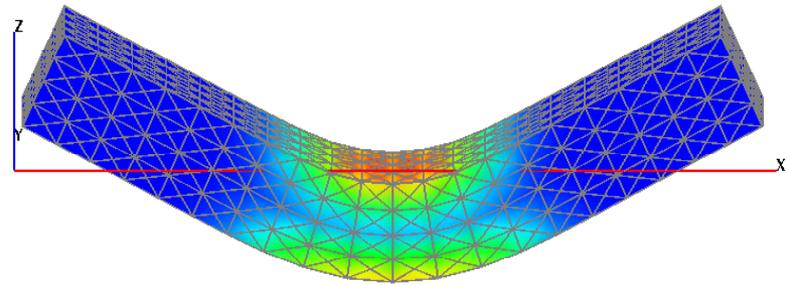
Material Anisotropy and Rate-Dependence

- Yield surface
 - $F(s_{ij}) - Y^2(e, T, \dots) = 0$
- Rate-dependence
- Code implementation
 - Antero, EPIC
- Physically-based
- Exp'r. characterization
 - Texture
 - Flow stress
- Applied to numerous materials



Polycrystal Plasticity

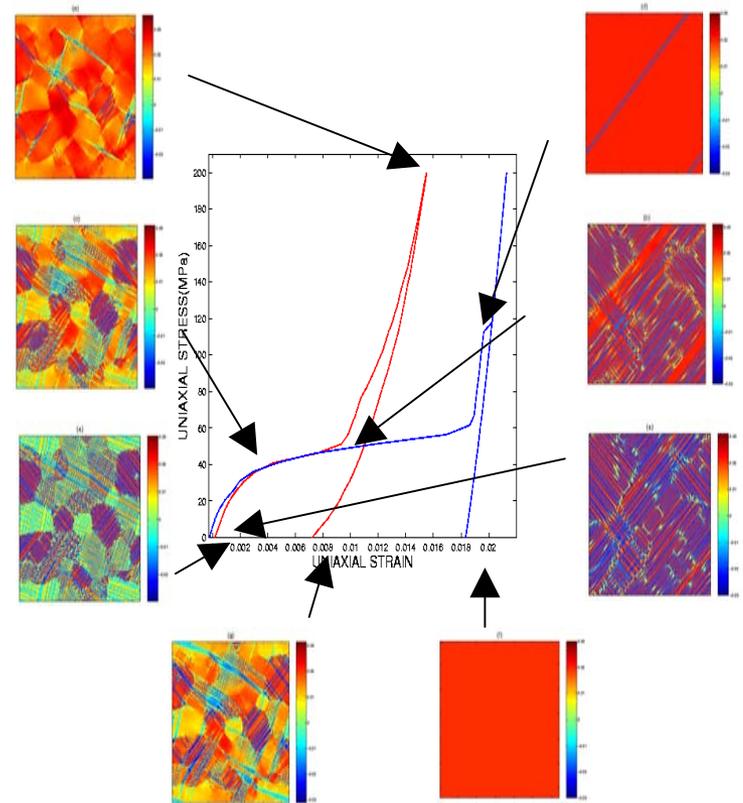
- VPSC Model
 - Texture
 - Hardening
 - Damage
 - Twinning
- Response to Strain Path Changes
- Low Sym. Matls.
 - Be, Zr, Mg
- Exp'r. Support
- Coupled to FEA



Meso-Scale Models

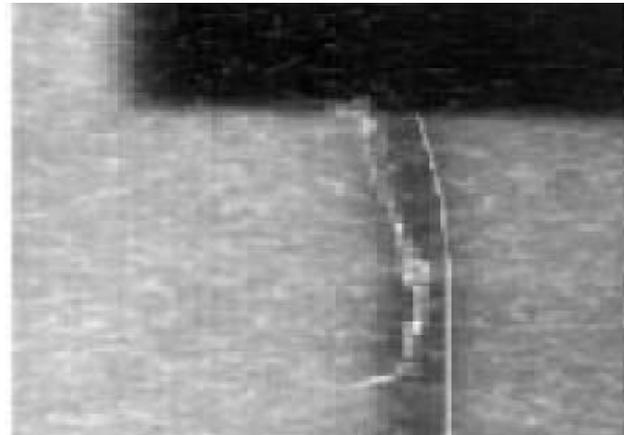
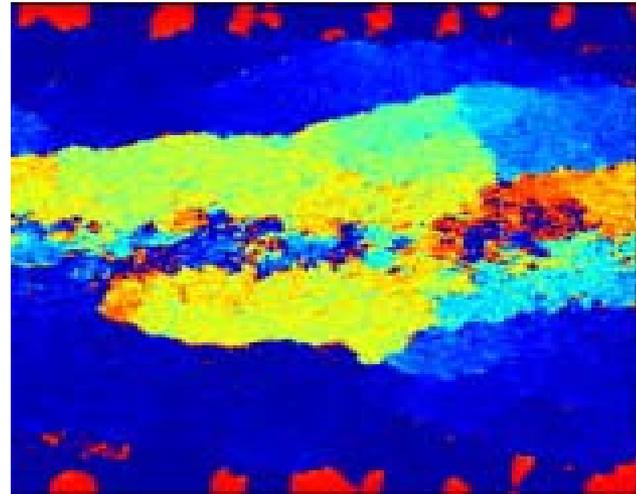
- Ginzburg-Landau
- Multivariant
- Single Crystal
- Polycrystal (VPSC)
- Homogenization

twinned martensite



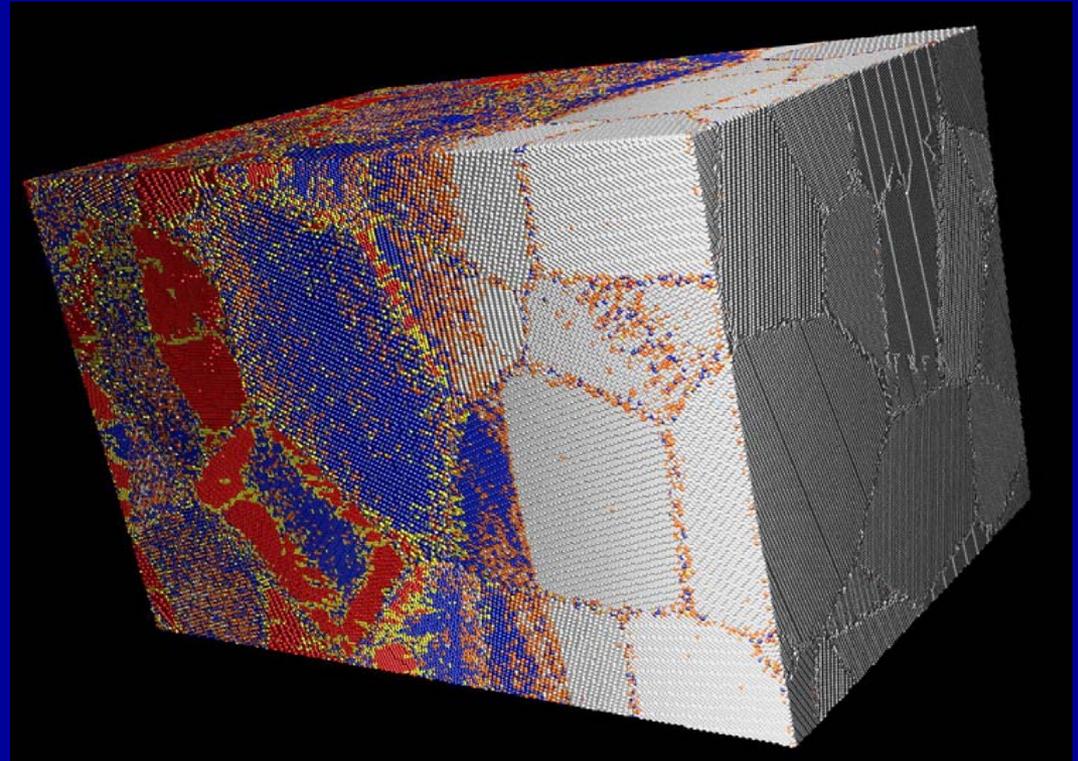
Interfacial Dynamics

- Interfacial sliding
- Micro-simulations
- Meso-simulations
- Comparison with experiment
- High shear velocities
- High pressure



Molecular Dynamics

- SPaSM
- Finite Range Potentials
- 10^8 particles
- Time Scale 10^{-11} s
- Length Scale nm
- Shock Physics
- Phase Transf.
- Nano Crystals
- Ejecta
- Surface Effects

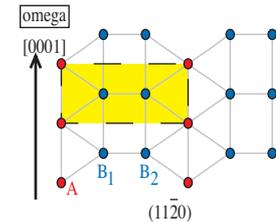
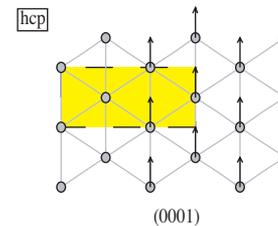


Applications of Tight-Binding Methods

- EOS calculations
- Phase stability and transformation paths
- Phonon
- Complex geometries (defects, grain boundaries, voids, ...)
- Diffusion barriers
- Materials aging
- Nonequilibrium materials properties
- Mechanical properties

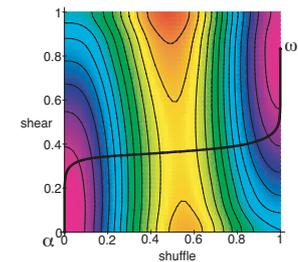
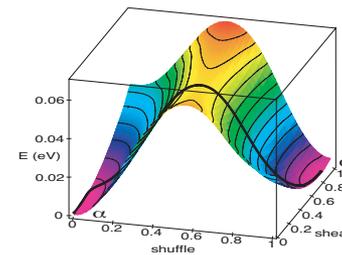
$\alpha \rightarrow \omega$ Pathway for Ti

- Simple α to ω pathway (Silcock)



- We can study the pathway by assuming a homogeneous atom shuffle with unit cell shear.

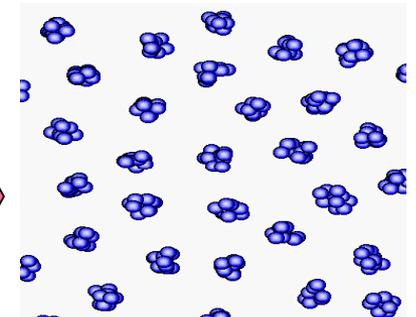
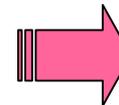
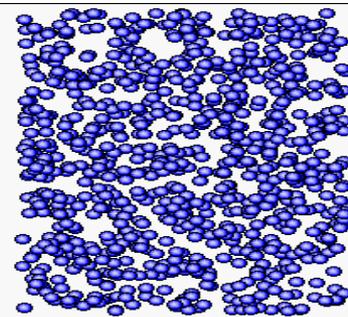
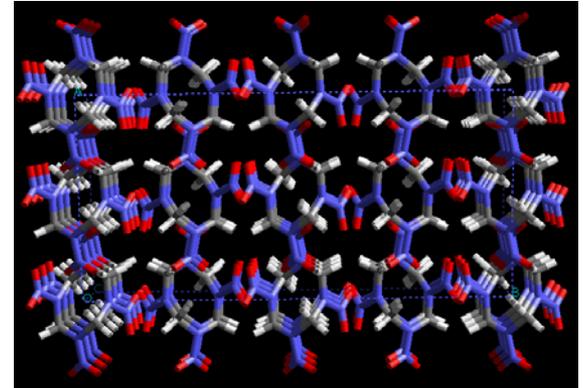
$E(\text{barrier}) = 49 \text{ meV}$



Quantum Chemistry / MEAM Simulations

- MondoSCF
 - Linear Scaling
 - Parallel
- Density Functional Theory
- Three-Dimensional, Periodic Bn'dy Conditions
- Large Scale (~1000 atoms)
- Shocked polymer MEAM simulation (20,000 atoms)

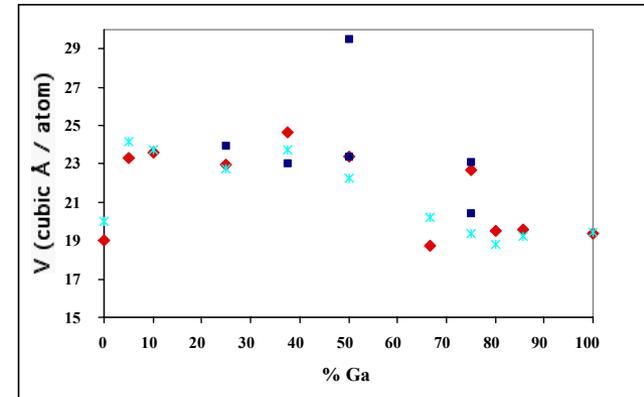
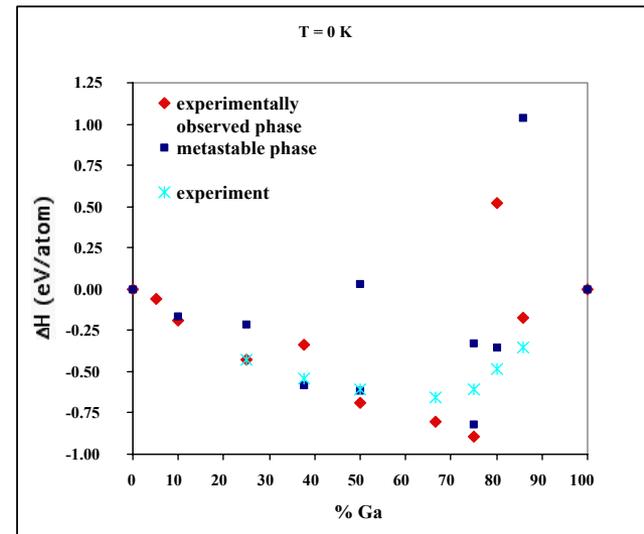
β -phase HMX



Decomposition of Polyethylene

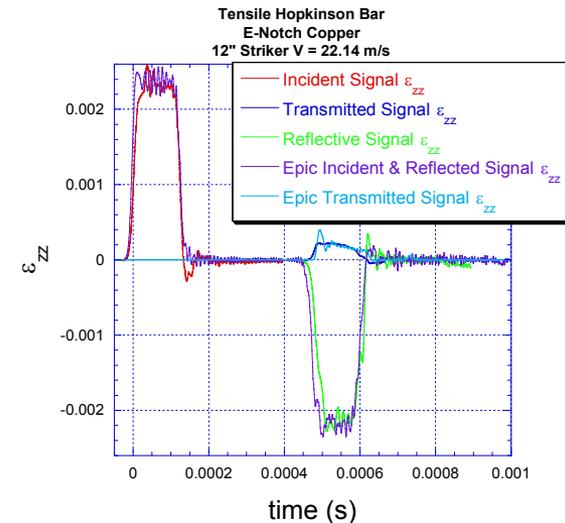
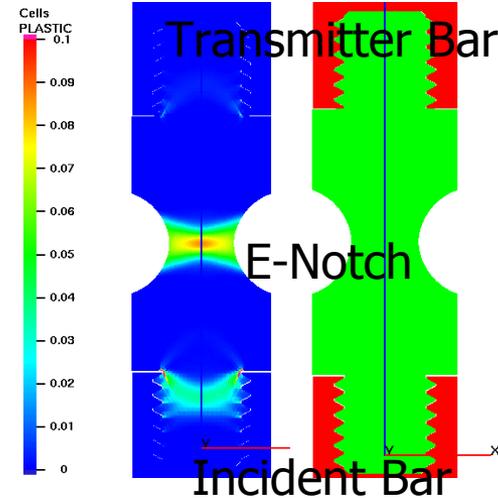
Modified Embedded Atom Method

- Develop MEAM potentials
- Predict energy and volume of stable phases / compare to experiment
- Insight into Pu-Ga phase diagram
- Understand phase transf. under shock loading
- Aging effects on phase stability
- Implement potentials into MD simulations



Model Validation

- Low-/High-Strain Rate
- Ten./Compr. Hoppy Bar
- Taylor Impact
- Plate Impact
- Notched Bar
- Microscopy
- Neutron Scattering



Sample of Planned Accomplishments

- Phase Diagrams / Properties
 - Improved Pu/Ga Potentials
 - Implementation of improved material moduli
- Interface Properties
 - MD interfacial simulations (friction, surface roughness)
- Mechanical Properties of HE
 - MD void collapse simulations (HE)
 - Accurate simulations of HE reactant & product mechanical properties
 - Accurate chemistry simulations of shock effects in non reactive & reactive diatomic systems (EOS)

Sample of Planned Accomplishments

- Elastic / Inelastic Deformations
 - Extended VPSC (twinning, texture, voids)
 - Meso-scale dynamic simulations to investigate grain size (1-100 nm) / yield strength effects
 - G.L. theory applied to U-Nb alloys
 - Improved potentials for inelastic strains (phase transf.,)
 - Flow stress enhancements (shock loading, twinning, ..)
- Dynamic Failure
 - Improved shear band model
 - Develop anisotropic damage potential
 - Implement brittle failure model into FEA
 - Tepla / SESAME link

Issues

- Experiment
 - Quantitative
 - Materials
 - Relevant Regimes
- Computer Methods
 - Lagrangian
 - Stable
 - User Friendly
- Multi-Code Support
 - Materials Interface
- Coordination
 - Programs
 - Groups / Divisions

Additional Funding

- Heterogeneous Materials
- Ejecta Formation
- Phase Transformation
- Improved Numerical Methods
- Code Implementation
- Materials Interface
- Formalize V & V

Summary

- Multi-Length Scale Approach
- Coupled to Experiment
- Multi-Divisional Effort
- Leveraged Program
- Excellent Scientific Effort
- Publications
- Collaborations
 - University
 - DOE / DoD Laboratories
 - Industry